Quantitative Assessment of Short-Ranged Chemical Order in High-Entropy Alloys

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ABSTRACT

The most distinctive feature of high-entropy alloys (HEAs) is that they form phases in which chemical elements are spread out on the same crystal lattice in an almost random manner. Yet, a small degree of local chemical order (LCO) exists and it is known to grant HEAs many of their distinctive properties. Characterization of LCO has been difficult to realize because of the sheer number of atomic configurations to be accounted for. For example, there are 3^(13) = 1,594,323 possible LCO configurations for each lattice site in the paradigmatic NiCoCr HEA. Furthermore, one could describe LCO as the tendency for some of these configurations to be a little more common than others (i.e., "slightly less random than completely random"), which does not translate easily into a physically intuitive and quantifiable picture. In this talk I will introduce an approach that combines fundamentals of statistical mechanics and information theory with machine learning techniques to quantify this incredibly large space of chemical configurations available for HEAs.

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